Bravais Lattice

A Bravais lattice is an infinite array of discrete points generated by a set of discrete translation operations. It describes the underlying geometric periodicity of a crystal.

Crucial Distinction: A Lattice is not a Crystal.

Lattice: Mathematical points in space.

Basis: The atom (or group of atoms) attached to every lattice point.

Crystal = Lattice + Basis.

A 3D Bravais lattice consists of all points with position vectors R of the form:

$$\mathbf{R} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}$$

- $Where: n1, n2, n3\ are\ integers.$
- $a1, a2, a3\ are\ the\ primitive\ translation\ vectors$. These vectors must be linearly independent (non-coplanar).

Types of Unit Cells:

To visualize the lattice, we define "cells" that repeat to fill space.

1) $Primitive\ Unit\ Cell(P)$:
   - $The\ \ smallest\ possible\ volume\ that\ can\ tile\ space.$
   - $Contains\ exactly\ 1\ lattice\ point(total).$
   - $Volume\ V\ = |\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})|$
2) Conventional Unit Cell:
   - A larger cell chosen to display the full symmetry of the lattice (e.g., a cube for FCC, even though the primitive cell of FCC is a rhombohedron).
   - May contain >1 lattice point.

3) Wigner-Seitz Cell:

A unique primitive cell constructed by taking a lattice point and drawing perpendicular bisectors to all its neighbours. The enclosed volume is the Wigner-Seitz cell.

The 4 Types of Centering

Lattices are classified by how "filled" their conventional unit cells are.

Symbol	Name	Description	Points per Cell
C	**Base-Centered**	Points at corners + 2 points at the centers of opposite faces (e.g., the xy faces). Sometimes called A- or B-centered depending on the axis.	**2**
P	**Primitive**	Points only at the 8 corners.	1
I	**Body-Centered**	Points at corners + 1 point in the exact center of the body.	2
F	**Face-Centered**	Points at corners + 6 points at the centers of all faces.	4

The 7 Crystal Systems and 14 Bravais Lattices:

I. Cubic System (Highest Symmetry)

- Parameters: a = b = c ; $\alpha = \beta = \gamma = 90^\circ$
- Lattices (3):
  1. Simple Cubic (SC): Primitive (P).Very rare (e.g., Polonium).
  2. Body-Centered Cubic (BCC): (I). Common in metals (Fe, Na, W).

3. Face-Centered Cubic (FCC): (F). Most efficient packing (Cu, Al, Au)

II. Tetragonal System (Stretched Cube)
- Parameters: $a = b \neq c$; $\alpha = \beta = \gamma = 90$
- Lattices (2):Simple Tetragonal (P)Body-Centered Tetragonal (I)

III. Orthorhombic System (Shoebox shape)
- Parameters: $a \neq b \neq c$; $\alpha = \beta = \gamma = 90$
- Lattices (4): (This system has the most variations)
  1. Simple Orthorhombic (P)
  2. Body-Centered Orthorhombic (I)
  3. Base-Centered Orthorhombic (C)
  4. Face-Centered Orthorhombic (F)

IV. Hexagonal System
- Parameters: $a = b \neq c$; $\alpha = \beta = 90°, \gamma = 120$
- Lattices (1):
  1. Simple Hexagonal (P)

Note: Many "hexagonal" metals are actually Hexagonal Close Packed (HCP).39 HCP is a lattice + a 2-atom basis, not a Bravais lattice on its own.

V. Trigonal (Rhombohedral) System
- Parameters: a = b = c ; $\alpha = \beta = \gamma \neq 90°$
- Lattices (1):
  1. Rhombohedral (R)

Note: Can often be described using a larger Hexagonal unit cell.

VI. Monoclinic System (Slightly skewed box)

Parameters: $a \neq b \neq$ C; $\alpha = \gamma = 90°, \beta \neq 90$

Lattices (2):

1. Simple Monoclinic (P)

2. Base-Centered Monoclinic (C)

VII. Triclinic System (General Parallelepiped)

Parameters: $a \neq b \neq c$; $\alpha \neq \beta \neq \gamma \neq 90$

Lattices (1):

1. Simple Triclinic (P) (Lowest symmetry, least constrained).